Exercise 3

Evaluate the eigenvalues and eigenvectors of the Hubbard Hamiltonian

$$\hat{H} = \begin{pmatrix} U & -t & t & 0 \\ t & 0 & 0 & -t \\ t & 0 & 0 & t \\ 0 & -t & t & U \end{pmatrix}$$

(a) What are the energy eigenvalues in the limit $t = 0$?
(b) How do these energy levels change as $t \neq 0$ in the limit $t/U << 1$?

Solution

The characteristic polynomial for the matrix is

$$\lambda^4 - 4\lambda^2 t^2 + 4\lambda t^2 U + \lambda^2 U^2 - 2\lambda^3 U$$

Leading to eigenvalues

$$\lambda_1 = 0 \qquad \lambda_2 = U \qquad \lambda_3 = \tfrac{1}{2}\left(U - \sqrt{U^2 + 16t^2}\right) \qquad \lambda_4 = \tfrac{1}{2}\left(U + \sqrt{U^2 + 16t^2}\right)$$

and corresponding eigenvectors

$$|0,1,1,0\rangle \qquad |-1,0,0,1\rangle \qquad \left|1, \tfrac{U+\sqrt{U^2+16t^2}}{4t}, -\tfrac{U+\sqrt{U^2+16t^2}}{4t}, 1\right\rangle \qquad \left|1, \tfrac{U-\sqrt{U^2+16t^2}}{4t}, -\tfrac{U-\sqrt{U^2+16t^2}}{4t}, 1\right\rangle$$

The diagonal matrix is

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & U & 0 & 0 \\ 0 & 0 & \frac{1}{2}W^- & 0 \\ 0 & 0 & 0 & \frac{1}{2}W^+ \end{pmatrix}$$

Where $W^+ = U + \sqrt{U^2 + 16t^2}$ and $W^- = U - \sqrt{U^2 + 16t^2}$

a) As $t \to 0$ $\quad W^+ \to 2U \quad W^- \to 0$ and the energy eigenvalues (leading diagonal) become

$$0 \qquad U \qquad 0 \qquad U$$

b) If $t/U << 1$

$$W^+ = U + U\Big(1 + 16(t/U)^2)^{1/2}\Big) \approx 2U + 8t^2/U$$
$$W^- = U - U\Big(1 + 16(t/U)^2)^{1/2}\Big) \approx -8t^2/U$$

and the energy eigenvalues are

$$0 \qquad U \qquad -4t^2/U \qquad U + 4t^2/U$$